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We have considered scattering rates and confined phonon modes in nitride-based confined nitride-based III-V heterostructures as well as the phonon modes in carbon nanotubes and buckyballs. We have examined phonons in a variety of nanostructures and related applications in optoelectronics, thin-films, thermal systems, nanotubes, and buckyballs. An especially significant finding of this research is the finding that quantized elastic continuum modes describe the acoustic phonon modes in nanostructures with a high degree of accuracy.

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SUBMITTED FOR PUBLICATION TO (applicable only if report is manuscript):

Michael A. Stroscio

Sincerely,

FINAL TECHNICAL REPORT ON
DAAG55-98-D-0003 (ARO 39108-EL-SR)
"Tailoring of Acoustic and Optical Phonon Modes in Mesoscopic and Nanoscale Semiconductor Structures"

(1) Foreword

We have considered scattering rates and confined phonon modes in nitride-based confined nitride-based III-V heterostructures as well as the phonon modes in carbon nanotubes and buckyballs. We have examined phonons in a variety of nanostructures and related applications in optoelectronics, thin-films, thermal systems, nanotubes, and buckyballs. An especially significant finding of this research is the finding that quantized elastic continuum modes describe the acoustic phonon modes in nanostructures with a high degree of accuracy.

(2) Table of Contents

(3) List of Appendixes --- N/A

(4) Statement of Problem Studied

The elastic and dielectric continuum models [1] have been applied widely to describe the properties of phonons in nanostructures. The authors of Reference 2 have formulated a universal continuum model that may be used to verify the appropriateness of simpler continuum models for specific applications. These models have been applied to describe phonons in quantum wells and superlattices, quantum wires and quantum dots, microtubulin structures found in biological systems, and intersubband lasers [1]. Moreover, such continuum models have been used to describe the damping of coherent acoustic phonon modes in quantum dots, the effect of phonon confinement on the properties of superconducting thin films, the Cerenkov generation of acoustic

phonons, and phonons in wurtzite-based quantum wells [1]. The procedures for determining the properties of confined optical modes in zero-, one-, and two-dimensional structures have been developed during the last two decades. As discussed previously [1, 2], one of the most striking differences between bulk phonon modes and those of dimensionally-confined phonons is the large difference between the optical-phonon frequency of the bulk optical-phonon mode for a quantum-well material and the actual energies of the high-frequency interface optical-phonon modes in the quantum well. In cubic materials, there is usually strong confinement of optical phonon modes [3]; however, as shown in this work, this is not the case for dimensionally-confined wurtzite structures [3]. In this work, we have demonstrated that the elastic continuum model may be applied to determine the frequencies of acoustic phonons even for one-monolayer-thick fullerenes and nanotubes.

(5) Summary of Most Important Results

Phonons in Dimensionally-Confined Wurtzite Structures

The dielectric continuum model provides a convenient formalism [1,3] for extending the traditional treatment of confined phonons in zinc blende structures to those in dimensionally-confined wurtzite systems. Such an extension yields confined phonon modes exhibiting greater dispersion than in the zinc blende case as a result of the anisotropy associated with the two distinct components of the dielectric tensor for the wurtzites: one along the c-axis, $\varepsilon_z(\omega)$, and the other in the plane normal to the c-axis, $\varepsilon_t(\omega)$. These dielectric constants must satisfy approximately the following condition: $\varepsilon_z(\omega)\cos^2\theta + \varepsilon_t(\omega)\sin^2\theta = 0$ [3]. The confined modes in wurtzite structures are found to be more complicated than the corresponding modes in crystals of cubic symmetry and it is found that propagating modes occur as a result of the significant overlap in the frequencies of the materials constituting the heterostructure. When the product of the parallel and perpendicular dielectric constants in a heterolayer is negative, oscillating phonon modes are allowed. Conversely, when this product is positive, the phonon modes are damped strongly. That is, $\varepsilon_t(\omega)\varepsilon_z(\omega) < 0$ and $\mathrm{Im}[\kappa_z] = 0$ for oscillating waves, and $\varepsilon_t(\omega)\varepsilon_z(\omega) > 0$ and $\mathrm{Re}[\kappa_z] = 0$ for decaying waves; here, κ_z is the z-component of the phonon wavevector, q. As a consequence, the so-called confined modes in the wurtzites exhibit greater dispersion than those of the zinc blende structures. In this research, we have considered [3] the wurtzite $Al_xGa_{1-x}N$/GaN/ $Al_xGa_{1-x}N$ quantum-well system with the c-axis normal to the heterointerfaces of the quantum well. The dispersion relations derived in this work show clearly that the so-called confined modes of the wurtzite system differ substantially from those of the zinc blende system; this occurs as a result of the greater overlap in the phonon frequencies associated with larger dispersions for the constituent uniaxial materials.

Phonons on Fullerenes and Nanotubes

As discussed previously [1], the quantization along the lengths of the quantum wires may be treated approximately under the simplifying "open" and "clamped" boundary conditions to assess the extent to which boundaries of nanoscale quantum wires influence the acoustic phonon modes in nanoscale devices. Indeed, it is this axial structure of the acoustic modes that determines the strengths of the deformation and piezoelectric scattering rates in wire-like structures. It is emphasized that the amplitudes of the acoustic phonons in quantum wires influence the electron--acoustic-phonon scattering rates in such nanoscale devices. For carbon nanotubes, the classical solution for the acoustic modes [4] of a thin-walled cylinder subjected to clamped boundary conditions at the ends of the finite-length cylinder, may be quantized according to the prescription of Ref. 4 to obtain the approximate acoustic mode amplitudes and dispersion relations. As described in Ref. 4, when clamped boundary conditions are imposed at the ends of the tube the transcendental equation --- $\tan(\mu l/2a) + \tanh((\mu l/2a) = 0$ --- is found to determine the discrete values of μ (the analog of the axially-directed wave vector, k_z, for a tube of finite length). We have published the solutions to this equation [4] for a 56-Angstrom-long nanotube with a 14-Angstrom diameter for the case where the nanotube is clamped such that the displacement is zero at each end. The lowest mode for both nanotubes has an energy of about 175 cm^{-1} over a range of wave vectors and corresponds to the analog of the 166-cm^{-1} breathing mode of a 14-Angstrom-diameter nanotube of infinite length. The elastic membrane mode of Ref. 5 has been applied as well to the case of a thin spherical shell [6]. By normalizing the amplitudes of Lamb's [6] original solutions [1] so that the energy in each mode is equal to the energy of the phonon, and using the elastic properties --- Young's modulus and Poisson's ratio --- of a graphene sheet, the energy of the elongation mode --- the b_2 mode of Lamb --- of a buckyball is readily determined to be 32 meV. This is in excellent agreement with 35 meV value determined experimentally by Park et al. [7] for the corresponding nanomechnical oscillation frequency of C_{60}. In conclusion, these results demonstrate that optical phonons in dimensionally-confined wurtzire ionic crystals are not confined as strongly as in the case of cubic ionic crystals. Moreover, it is demonstrated that the elastic continuum model of acoustic phonons provides excellence predictions of the acoustic mode frequencies even for one-monolayer-thick fullerenes and nanotubes.

(6) List of Publications and Technical Reports

S. M. Komirenko, K. W. Kim, M. A. Stroscio, and M. Dutta, "Energy- Dependent Electron Scattering via Interaction with Optical Phonons in Wurtzite Crystals and Quantum Wells," Phys. Rev., B61, 2034 (2000).

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(7) List of All Participating Scientific Personnel

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Daniel Kahn
Sergiy Komirenko, received his PhD, in part, for research supported under this program

(8) Report of Inventions: None

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(10) Appendixes --- None